

Open Problems in Applying Random-Matrix Theory to Nuclear Reactions

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Abstract.

Problems in applying random-matrix theory (RMT) to nuclear reactions arise in two domains. To justify the approach, statistical properties of isolated resonances observed experimentally must agree with RMT predictions. That agreement is less striking than would be desirable. In the implementation of the approach, the range of theoretically predicted observables is too narrow.

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1. Purpose

Nuclear Reactions on medium-weight and heavy target nuclei in the low-energy domain (bombarding energies up to several tens of MeV) are dominated by compound-nucleus (CN) resonances. An adequate reaction theory requires information on the spins, parities, partial and total widths and on the spacings of these resonances. With typical resonance spacings d (for fixed quantum numbers) in the 10 eV range even at neutron threshold (and with very much smaller values of d at higher excitation energies), nuclear-structure theory cannot supply such information. The necessary calculations are beyond present-day capabilities. In its stead one follows Wigner's [1, 2] original proposal and uses random-matrix theory (RMT). RMT in its time-reversal invariant form (the Gaussian Orthogonal Ensemble (GOE)) has become a standard tool of nuclear reaction theory [3, 4].

We ask: What are the problems and challenges in applying the GOE to nuclear reactions? The question has two parts. (i) Are the properties predicted by the GOE consistent with experimental data on CN resonances? (ii) Is it possible to implement the GOE into a viable and useful theory of nuclear resonance reactions? An affirmative answer to question (i) is the necessary condition for a physically meaningful use of RMT in nuclear reaction theory. Asking that question is particularly timely. Refs. [5, 6, 7] reported strong disagreement of neutron resonance data with GOE predictions. Some of these results have found wide attention [8, 9, 10, 11] eroding, as they seemingly do, one of the cornerstones of the statistical theory of nuclear reactions [3, 4]. After defining the GOE in Section 2 we address questions (i) and (ii) in turn.

2. The GOE

The GOE is an ensemble of Hamiltonian matrices H in N -dimensional Hilbert space. Because of time-reversal invariance, the matrices H are real and symmetric. The ensemble is defined in terms of the probability density

$$\mathcal{P}(H)dH = \mathcal{N}_0 \exp \left\{ -\frac{N}{4\lambda^2} \text{Tr}(H^2) \right\} dH. \quad (1)$$

Here \mathcal{N}_0 is a normalization constant, λ is a parameter of dimension energy which (in the center of the GOE spectrum) is related to the mean level spacing d by $d = \pi\lambda/N$, and

$$dH = \prod_{\mu \leq \nu}^N dH_{\mu\nu} \quad (2)$$

is the product of the differentials of the independent matrix elements. Eq. (1) shows that the independent elements of H are uncorrelated Gaussian-distributed random variables. Eqs. (1) and (2) show that the ensemble is invariant under orthogonal transformations of Hilbert space. Hence its name Gaussian Orthogonal Ensemble.

Every matrix H can be diagonalized by an orthogonal transformation \mathcal{O} . The eigenvalues are denoted by E_μ with $\mu = 1, \dots, N$. In terms of these variables the

distribution takes the form

$$\mathcal{P}(H)dH = \mathcal{N}_0 d\mathcal{O} \exp \left\{ -\frac{N}{4\lambda^2} \sum_{\mu} E_{\mu}^2 \right\} \prod_{\rho < \sigma} |E_{\rho} - E_{\sigma}| \prod_{\nu} dE_{\nu} . \quad (3)$$

The factor $d\mathcal{O}$ is the Haar measure of the orthogonal group in N dimensions and defines the distribution of eigenvectors. It implies that in the limit $N \rightarrow \infty$ the projections of all eigenvectors onto any fixed vector in Hilbert space are Gaussian-distributed real random variables. The factor $\prod_{\rho < \sigma} |E_{\rho} - E_{\sigma}|$ causes the linear level repulsion characteristic of the GOE. The distribution (3) factorizes, one factor depending only on the eigenvectors and the other, only on the eigenvalues. Hence, eigenvectors and eigenvalues are statistically independent. This result follows directly from the orthogonal invariance of the GOE.

Theoretical predictions of the GOE for spectral fluctuations (Section 3) and for cross-section fluctuations (Section 4) are based on ensemble averages. These are compared with experimental data obtained by taking the running average over energy of a single spectrum. For the GOE it has been shown (albeit only for a restricted set of observables) that the ensemble average and the running average taken over the spectrum of a single member of the GOE agree. This fact is the basis for comparison with experimental data. To minimize the statistical error, long data sequences are required.

According to the Bohigas-Giannoni-Schmit conjecture [12], the spectral fluctuation properties of dynamical systems that are chaotic in the classical limit agree with RMT predictions. Therefore, the applicability of the GOE to nuclear reaction theory is linked to the question whether the nuclear dynamics is chaotic. We do not discuss here general tests relevant to that question (such as the spacing distribution of levels in the ground-state domain, or of levels some 100 keV above the yrast line, or of the eigenvalues of the interacting boson model). The dynamics of such low-lying excitations do not have any immediate bearing on nuclear reaction theory.

3. Tests of GOE Spectral Fluctuations in Nuclei

Three basic predictions of the GOE can be tested: (i) the distribution of level spacings as obtained from the last three factors in Eq. (3) in the limit $N \rightarrow \infty$; (ii) the Gaussian distribution of eigenvectors deduced in the same limit, (iii) the independence of the distributions of eigenvectors and eigenvalues. Significant tests have been done either on data generated by large-scale shell-model calculations, or on experimental data obtained from the analysis of sequences of isolated resonances. To be statistically significant, the data sets should be large, each set should be clean (the quantum numbers of all resonances should be unambiguously known and be identical), and the sets should be complete (no resonances missing). The three requirements are difficult to fulfill experimentally (long sequences are hard to come by, very narrow resonances are easily missed, unambiguous spin assignments may be very difficult to obtain). In spite of 60 years of work on the problem, the experimental data sets that fulfill these requirements

are, therefore, small in number. Results of shell-model calculations have been extensively tested for GOE properties only for $s - d$ -shell nuclei.

3.1. Level-Spacing Distribution

Two measures are mainly used to test GOE predictions for the level-spacing distribution: Wigner’s surmise for the nearest-neighbour spacing (NNS) distribution, and the Δ_3 statistic of Mehta and Dyson. The NNS distribution gives the distribution of spacings of neighbouring eigenvalues. It accounts mainly for level repulsion and not for long-range correlations of spacings. It is not a very sensitive test of general GOE properties. Numerical studies of few-degrees-of-freedom systems with varying interaction strength have shown that level repulsion sets in quite early and before all other GOE properties are attained. The Δ_3 statistic is more sensitive as it measures long-range correlations of level spacings. It requires long sequences of data.

Results of shell-model calculations for $s - d$ -shell nuclei were tested for agreement with GOE predictions in Ref. [13]. Both the NNS distribution and the Δ_3 statistic were calculated for the 3276 states with spin $J = 2$ and isospin $T = 0$ that occur in the middle of the shell. In both cases, agreement with the GOE is very good, except that the Δ_3 statistic has a tendency to lie slightly above the GOE curve for very large lengths L . That tendency seems not fully understood. The agreement is expected. It is due to the (almost) complete mixing of shell-model configurations in eigenstates of the shell-model Hamiltonian that are near the center of the spectrum. To be sure, the mixing addressed in Ref. [13] refers only to the configurations within a single major shell. Shell structure being manifest over a wide range of excitation energies, one may wonder what happens at excitation energies that lie in the middle between two major shells. That question seems not to have been addressed in the theoretical literature. With this proviso, it is theoretically expected that CN resonances follow the GOE.

Relevant experimental information comes from the analysis of isolated resonances measured in the scattering of slow neutrons on medium-weight and heavy nuclei and, with a smaller data set, from scattering of protons on medium-weight nuclei at energies near the Coulomb barrier. For neutrons scattered on even-even nuclei, all s -wave resonances have spin/parity assignment $1/2^+$ while p -wave resonances carry spin-parity assignments $1/2^-$ and $3/2^-$. Because of the angular-momentum barrier, the latter are suppressed by a factor E (the resonance energy measured from threshold) relative to the former. Spin-parity assignments for resonances in proton scattering are frequently less problematic. Most available sequences of resonances being quite short, Haq, Pandey and Bohigas [14] in the 1980’s combined resonance data from a number of nuclei into the “Nuclear Data Ensemble” (NDE). The NDE comprises 30 sequences of levels of 27 different nuclei amounting to a total of 1407 resonance energies [14]. Up to this day, the NDE or a suitable modification that takes into account more recent data has been the backbone of work on the level-spacing distribution.

Under the (tacit) assumption that all neutron resonances in the NDE have

spin/parity assignment $1/2^+$ (i.e., no p -wave admixtures), it was shown in Ref. [14] that the data were in good agreement with the Δ_3 statistic for sequence lengths $L \leq 20$. In Ref. [15] the analysis was extended to the NNS distribution (resulting in good agreement with the Wigner surmise), and to the Porter-Thomas distribution (discussed below) for neutron widths. The Δ_3 statistic is determined by the two-level correlation function. Measures accounting for the three- and four-level correlation functions were evaluated for the NDE and compared with GOE predictions in Ref. [16], again resulting in good agreement. A further test [17] involving higher n -point functions uses the fact that omission of every other level in a GOE spectrum yields a GSE spectrum (the GSE is the Gaussian symplectic ensemble of random matrices). In applying that test to the NDE, “no disagreement with the GOE” could be detected [17]. Taken together, the work of Refs. [14, 15, 16, 17] yielded very strong evidence for the agreement of nuclear spectral fluctuations with GOE predictions.

The only existing test for correlations between eigenvalues and eigenfunctions seems to be the one in Ref. [17]. The NDE gave no evidence for such correlations, in agreement with the GOE.

One cause of uncertainty in the data analysis described so far is due to the possible presence of p -wave resonances in low-energy neutron scattering data. It is clear that firm and unbiased conclusions can only be drawn if s -wave and p -wave neutron resonances are cleanly separated. The problem was emphasized by Koehler who reconstructed and reanalysed the NDE [6]. Reconstruction was necessary because a full account of the analysis in Refs. [14, 15] of the NDE was never published, and because some of the references therein were based on private communication. The reconstructed NDE contains 1245 resonances and is not completely identical with the original one. A significant fraction (typically 5 – 10 percent) of the neutron resonances are of unknown parity or known to be p wave.

The Δ_3 statistic for the reconstructed NDE was analysed in Ref. [7]. Upon first sight, agreement with the GOE is obtained. The Δ_3 statistic using all nuclei in the reconstructed NDE agrees with the GOE, confirming the conclusion of Ref. [14]. Moreover, the Δ_3 statistic for the two nuclides with the longest level sequences (U and Th nuclei) also agrees with the GOE. However, for the remaining nuclei in the reconstructed NDE (U and Th nuclei omitted) the Δ_3 statistic deviates increasingly with increasing length L from the GOE prediction, the deviation becoming significant for lengths $L > 20$ or so. A similar deviation is found when resonances with a definite p -wave assignment are removed. These are mainly resonances in U and Th. It is concluded that contrary to the first impression, the Δ_3 statistic for the reconstructed NDE is in serious disagreement with the GOE.

Taken by themselves, the results on the Δ_3 statistic in Ref. [7] suggest rejection of the GOE hypothesis. In its entirety, however, work on the level-spacing distribution suggests a different conclusion. The test of the Δ_3 statistic in Ref. [14] was confined to sequence lengths $L \leq 20$. In that domain both Ref. [14] and Ref. [7] show full agreement with GOE predictions. The higher-order correlations tested in Refs. [16, 17]

also agree with the GOE. It is very difficult to see how such agreement could survive the admixture of p -wave resonances, or be accidental. For instance, it appears extremely unlikely that a sequence of s -wave resonances with some accidental admixture of p -wave resonances would, upon omission of every second resonance, obey GSE statistics. Given these facts we are left with the disagreement with GOE predictions found in Ref. [7] for the Δ_3 statistic and for sequence lengths $L > 20$. Here several questions come to mind. (i) Table I of Ref. [6] shows that the number of sequences with $L > 20$ decreases strongly with increasing L . Estimates of the statistical uncertainty of the Δ_3 statistic in Ref. [7] do not seem to reflect that fact. (ii) It is known that with increasing distance from neutron threshold, an increasing number of narrow resonances is missed experimentally. The remaining resonances lack the stiffness of the spectrum and are, therefore, expected to be more random. The resulting deviations of the Δ_3 statistic from the GOE prediction should tend towards the Poisson distribution. This is what the data show. (iii) Before removal of the supposed p -wave resonances, the Δ_3 statistic for U and Th agrees with the Δ_3 statistic for the GOE. After removal of these resonances, the Δ_3 statistic for the remaining s -wave resonances does not. It would take a very subtle correlation between s -wave and p -wave resonances to re-establish GOE properties in the combined sequence when the s -wave resonances alone lack such properties. The accidental occurrence of such a correlation seems utterly improbable. A dynamical correlation is excluded because states with different quantum numbers do not interact and, thus, lack the mechanism that would cause stiffness of the combined spectrum. An erroneous p -wave assignment to the excluded resonances seems to offer the most likely explanation.

3.2. Width Distribution

The partial-width amplitude of a CN resonance is proportional to the overlap of the resonance wave function with the channel wave function. In the RMT approach the resonance wave function is an eigenfunction of the GOE. Then, the partial-width amplitude is the projection of a GOE eigenvector onto some fixed vector in Hilbert space. Therefore, the GOE predicts that the partial-width amplitudes of CN resonances have a Gaussian distribution. Such amplitudes can only be measured in special cases. Relevant information comes mainly from neutron widths of isolated CN resonances measured in slow neutron scattering. The neutron width being the square of the neutron partial-width amplitude, its distribution is predicted to be the Porter-Thomas distribution (PTD) (a χ^2 distribution with a single degree of freedom, $\nu = 1$).

The shell-model calculations [13] referred to above for states with $J = 2$ and $T = 0$ in the middle of the s - d -shell have also been tested for comparison with GOE predictions for the eigenfunctions. Good agreement was found. That is another demonstration of the (nearly) complete mixing of shell-model configurations caused by the residual interaction. As in the case of the spectral fluctuations, the theoretical expectations are that GOE predictions apply to CN resonance eigenfunctions.

Experimental data on partial-width amplitudes come from proton scattering on medium-weight nuclei at energies near the Coulomb barrier, those on partial widths from data on isolated CN resonances in slow neutron scattering.

A very thorough test of the postulated Gaussian distribution of partial-width amplitudes was reported in Ref. [19]. Data on proton scattering by medium-weight nuclei yielded 1117 reduced partial-width amplitudes. If the amplitudes have a Gaussian distribution, the linear correlation coefficient of the squares of the amplitudes must be equal to the square of the correlation coefficient for the amplitudes. The positive test [19] provides strong support for the Gaussian distribution.

In the original analysis of the NDE, the distribution of neutron widths showed good agreement with the PTD [15]. As in the case of the level distribution, it is important to ascertain that all levels included in the analysis are s -wave resonances. A method to exclude p -wave resonances (as well as to avoid s -wave resonances with very small widths that partly escape experimental detection anyhow) in neutron resonance data was introduced in Ref. [20]. With E the resonance energy counted from threshold, s -wave (p -wave) resonances have an intrinsic energy dependence $E^{1/2}$ ($E^{3/2}$, respectively). The transition to reduced widths removes the $E^{1/2}$ dependence of the s -wave resonances and leaves a linear E dependence of the p -wave resonances. The latter (and all very narrow s -wave resonances) were removed by a cutoff. Only resonances with widths larger than the cutoff were retained. For a set of 9 nuclides the cutoff was chosen differently for each nucleus and in each case amounted to less than 10 percent of the average width. A maximum-likelihood (ML) analysis was used to test whether the remaining data were in agreement with the PTD. The likelihood function was dependent on ν , the number of degrees of freedom of a χ -squared distribution, and on the average width $\langle\Gamma\rangle$. For each nucleus, both ν and $\langle\Gamma\rangle$ were determined by the maximum of the likelihood function. The resulting values of ν were found to depend on the cutoff and, for the set of 9 nuclides, ranged from 0.64 ± 0.28 to 1.32 ± 0.30 , with an error-weighted mean value $\nu = 0.98 \pm 0.10$. In Ref. [20] that result was considered to be “completely consistent with the PTD”.

In the ML analysis of the width distribution for the reconstructed NDE in Ref. [6], a modified version of the cutoff procedure introduced in Ref. [20] was employed. A linearly energy-dependent cutoff was used. That cutoff safely removes all p -wave resonances. In addition, it simulates the experimental tendency to miss with increasing energy an increasing number of narrow s -wave resonances. The ML analysis [20] gave ν values for the individual nuclides (denoted by ν_{pf} in Table I of Ref. [6]) that range widely from $0.49(+0.64, -0.48)$ to $3.6(+1.6, -1.3)$. The resulting weighted average is $\nu = 1.217 \pm 0.092$. This result rejects the PTD with a statistical significance of at least 98.17 percent.

The same approach was used in Ref. [5] to analyse a set of neutron resonance data in the Pt nuclei (158 resonances for ^{192}Pt , 411 resonances for ^{194}Pt). The ML analysis with a cutoff yields very small ν values ($\nu = 0.47$ for ^{192}Pt , $\nu = 0.60$ for ^{194}Pt). When combined, these results reject agreement with RMT with a statistical significance of

at least 99.997 per cent probability [5]. These results caused some theoretical activity. However, none of the suggestions put forward in Refs. [9, 10, 11] seems able to remove that discrepancy [21] with the GOE.

The conclusions in Refs. [5, 6] are based on the ML analysis with a cutoff. How reliable is that method? In Ref. [22] the question is addressed both analytically and with the help of computer simulations. Starting point is the PTD with unit width. A fictitious ensemble of neutron widths is generated by drawing N widths randomly from the PTD, and by repeating the procedure 2500 times. By construction, these widths follow the PTD. The data are analysed with the help of an ML function with a cutoff. The procedure does not generate resonance energies so the cutoff chosen is constant. For each member of the ensemble, the maximum of the ML function yields a value for ν . The distribution of the resulting ν values over the ensemble is investigated numerically. For a cutoff of 0.1 (10 percent of the average width) and $M = 100$, the histogram for the distribution resembles a Gaussian centered at $\nu \approx 1$. The full width at half maximum is approximately unity. The combined error due to cutoff and finite M value is, thus, much bigger than the typical error estimated from the width of the maximum of the ML function for a single member of the ensemble. In Ref. [22] the origin of that error and its substantial growth with increasing cutoff are displayed. As a result, the ML analysis of a single set of widths drawn from a PTD may yield a value for ν that differs widely (by $\pm 1/2$ or so) from the actual value $\nu = 1$.

In the light of these results, it is not clear whether the two small ν values found in Ref. [5] are inconsistent with the GOE. Moreover, it is conceivable that the spread of ν values found for a set of nuclides in Ref. [20], and for the reconstructed NDE in Ref. [6], both reflect the width of the distribution of ν values due to cutoff and finite sample size. It appears that definite conclusions on the validity of the GOE hypothesis can be drawn only when every ML analysis using a cutoff is supported by simulations of the type used in Ref. [22].

In summary, there is substantial theoretical [13] and experimental [19] evidence in favour of a Gaussian distribution of partial-width amplitudes. The case of neutron widths [5, 6] is unresolved.

4. Implementation of the GOE for Nuclear Reactions

We turn to question (ii) raised in Section 1: How is it possible to implement the GOE into a viable and useful theory of nuclear resonance reactions? In the standard approach and in the absence of direct reactions, the symmetric and unitary scattering matrix is written as [3, 4]

$$S_{ab}(E) = \delta_{ab} - 2i\pi(W^\dagger D^{-1}(E)W)_{ab} \quad (4)$$

where

$$D_{\mu\nu}(E) = E\delta_{\mu\nu} - H_{\mu\nu} + i\pi(WW^\dagger)_{\mu\nu} . \quad (5)$$

Here E is the energy. The indices a, b (μ, ν) denote the Λ open channels (the N states of the GOE, respectively). The Hamiltonian H is a member of the GOE defined in Section 2. The matrix W is rectangular. The elements $W_{\mu a}$ couple the GOE states to the channels. Because of time-reversal invariance, the $W_{\mu a}$ are real so that $W_{\mu a} = W_{a\mu}$, they are independent of energy E , and they obey $(W^\dagger W)_{ab} = \delta_{ab} N v_a^2$. The last condition guarantees diagonality of the average S matrix, i.e., absence of direct reactions. The form of S in Eqs. (4, 5) seems uncontroversial and generally accepted. The same is true for a more general form of S that allows for the presence of direct reactions [3, 4]. Equivalent forms (where S is written in terms of the K matrix) are also commonly used. In the limit $N \rightarrow \infty$ the number of parameters of the GOE approach is Λ : the spacing parameter λ and the Λ parameters v_a^2 for the coupling strengths to the channels are combined to yield Λ dimensionless parameters v_a^2/λ . That number is equal to the number of diagonal average S -matrix elements. The latter serve as input for the prediction of S -matrix fluctuation properties.

The number Λ of open channels in Eqs. (4, 5) is considered fixed. With increasing energy, the number of open channels in any nuclear reaction actually increases exponentially. Therefore, Eqs. (4, 5) provide a useful approximation to S only within some finite energy interval ΔE . The interval is defined by the condition that the coupling of GOE states to all channels with thresholds within ΔE is sufficiently weak. Under that condition the neglect of the energy dependence of the matrix W is also justified. The assumption is most strongly violated by s -wave neutron channels because here neither angular momentum barrier nor Coulomb barrier suppress the coupling to the GOE states. It seems that the number of such cases that are experimentally relevant, is small. Their adequate theoretical treatment would pose a problem.

In principle, Eqs. (4) and (5) can be used to predict theoretically correlation functions (as ensemble averages) involving products of two or more S -matrix elements. Because of the technical difficulties in the calculation of such averages, the predictive power of the GOE for nuclear reactions is actually much more limited than for spectral fluctuations. General analytical results exist only for the correlation function involving a pair of S -matrix elements [23], for select values of the correlation function involving three or four S -matrix elements [24, 25], and for the probability distribution of single S -matrix elements [26, 27, 28, 29]. The complete joint probability distribution of all S -matrix elements is known [30, 31, 32] only in the Ericson regime (strongly overlapping resonances). From a practical point of view, results beyond average cross sections and beyond the Ericson regime, especially for cross-section correlation functions, would be of considerable interest. The theoretical treatment of direct reactions (non-zero values of non-diagonal average S -matrix elements) does not seem to pose a problem.

5. Summary

The problems in applying random-matrix theory to nuclear reactions lie in two domains.

(i) In the justification of the approach. Such justification must be based upon established

statistical properties of isolated resonances. The data base is narrow. In general, the data agree with GOE predictions. Open questions exist for the Δ_3 statistic for long sequences of levels, and for the distribution of neutron widths. (ii) In the implementation of the approach. The range of theoretically predicted observables has grown in recent years but is still too narrow. Theoretical expressions for cross-section correlation functions would be particularly valuable.

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